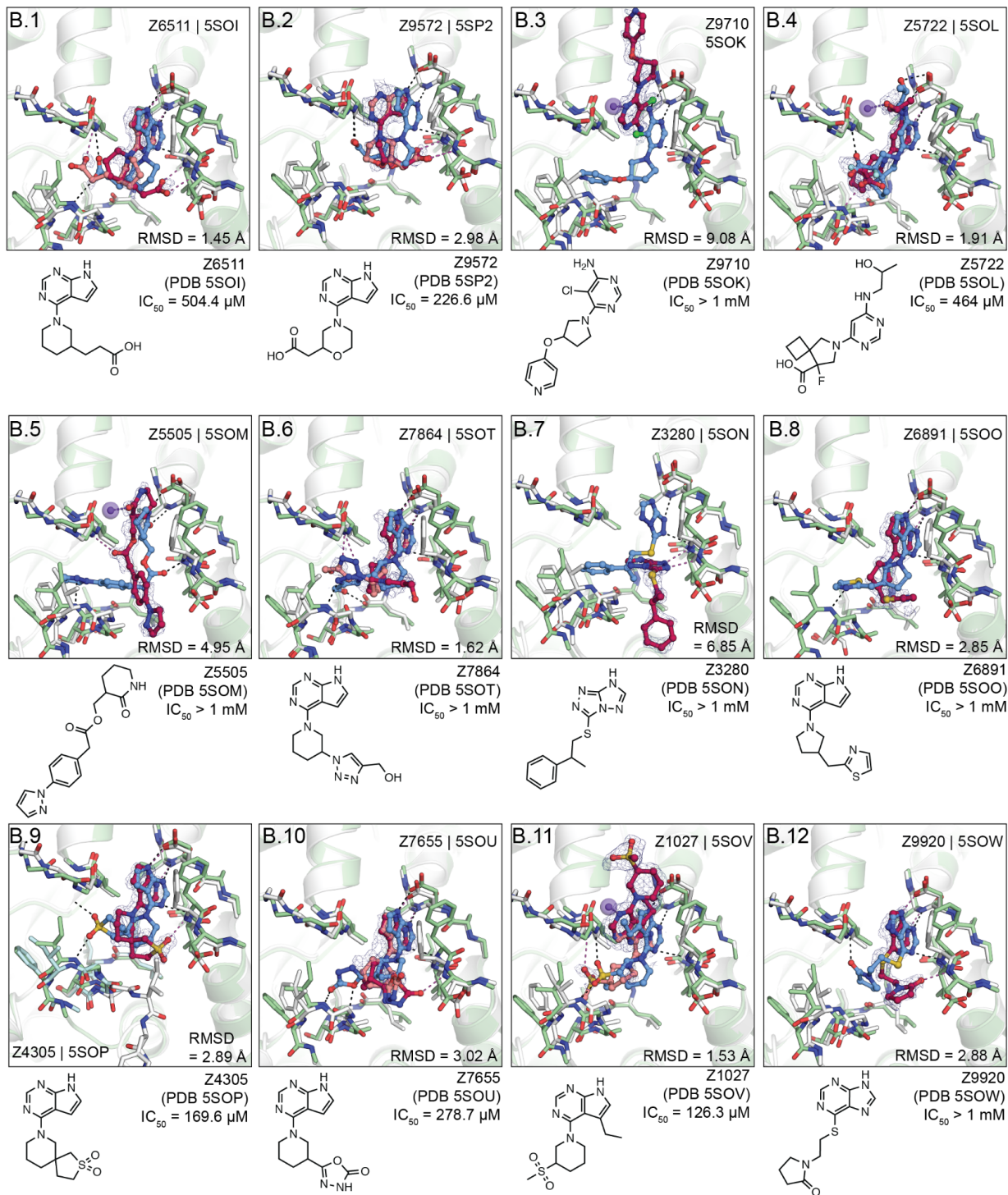


**Dataset S4:** Crystal structures of Mac1 in complex with docking hits. PanDDA event maps are shown for ligands (contoured at  $2\sigma$ ). Protein-ligand hydrogen bonds are shown with dashed black lines. Hydrogen bonds between ligands and the Lys11 backbone nitrogen of a symmetry mate are highlighted with purple spheres/dashes.

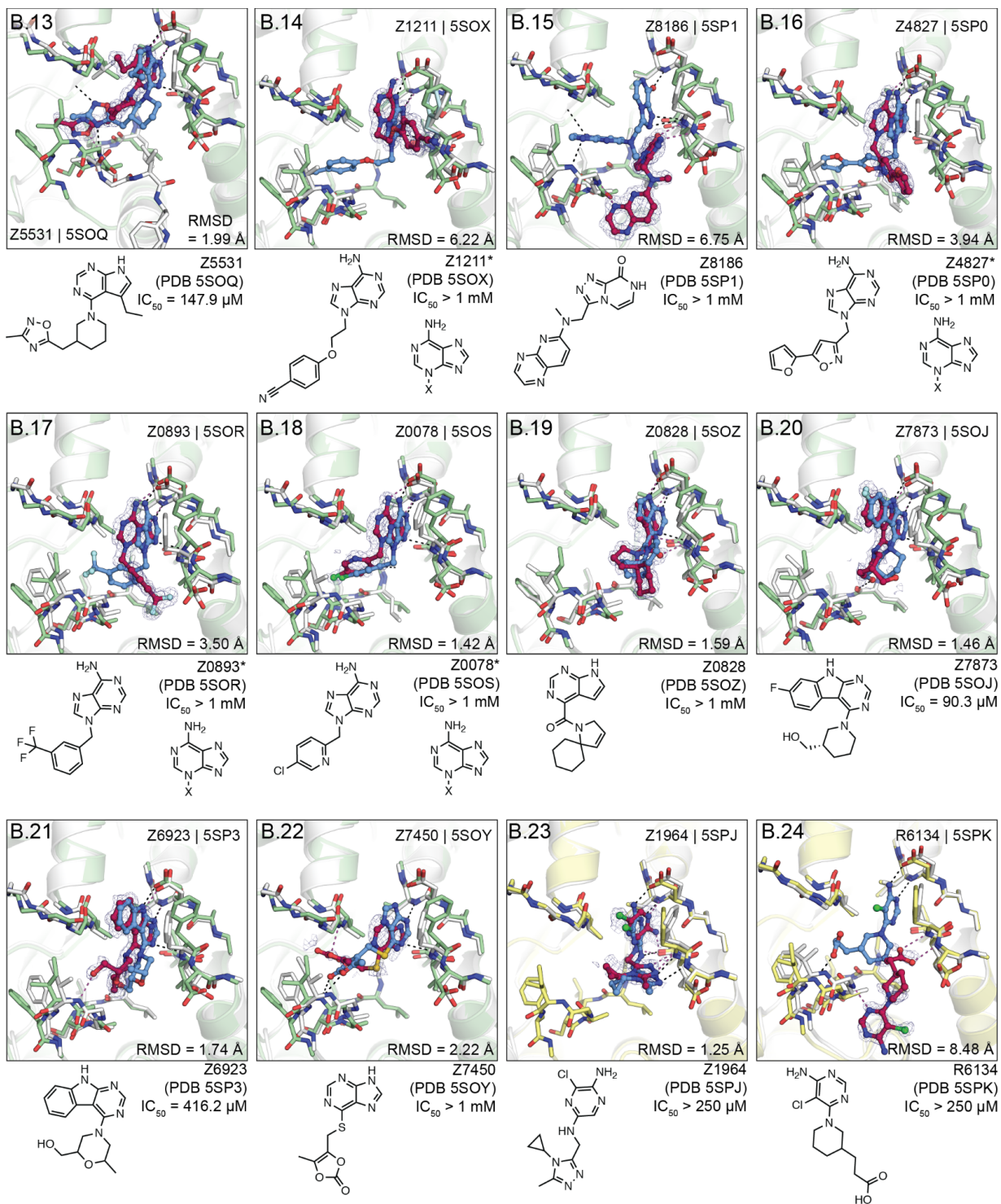


1<sup>st</sup> Screen Docking Template

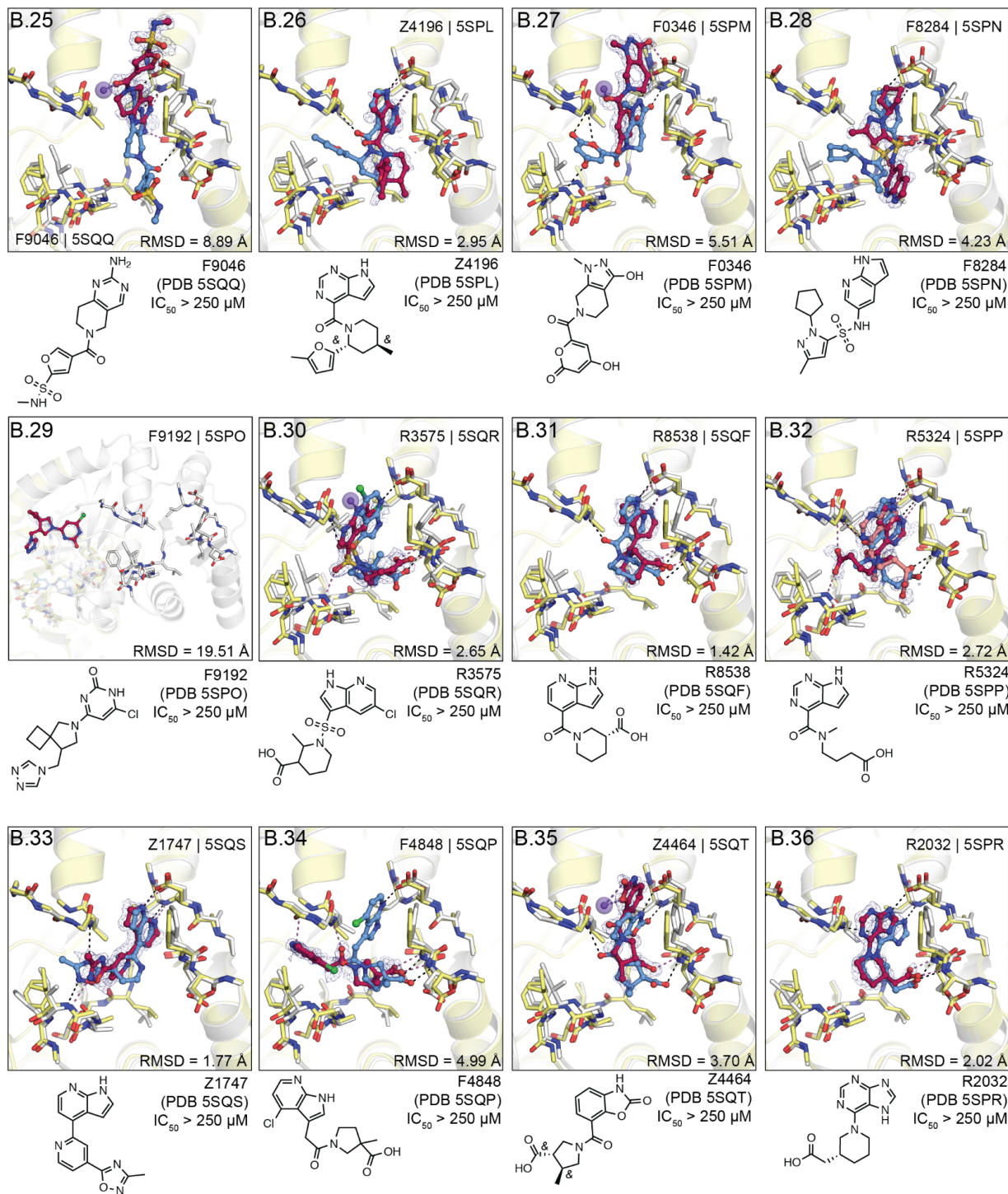
Docking Prediction

Crystal Structure

Solved Pose



1<sup>st</sup> Screen Docking Template | 2<sup>nd</sup> Screen Docking Template | Docking Prediction | Crystal Structure | Solved Pose

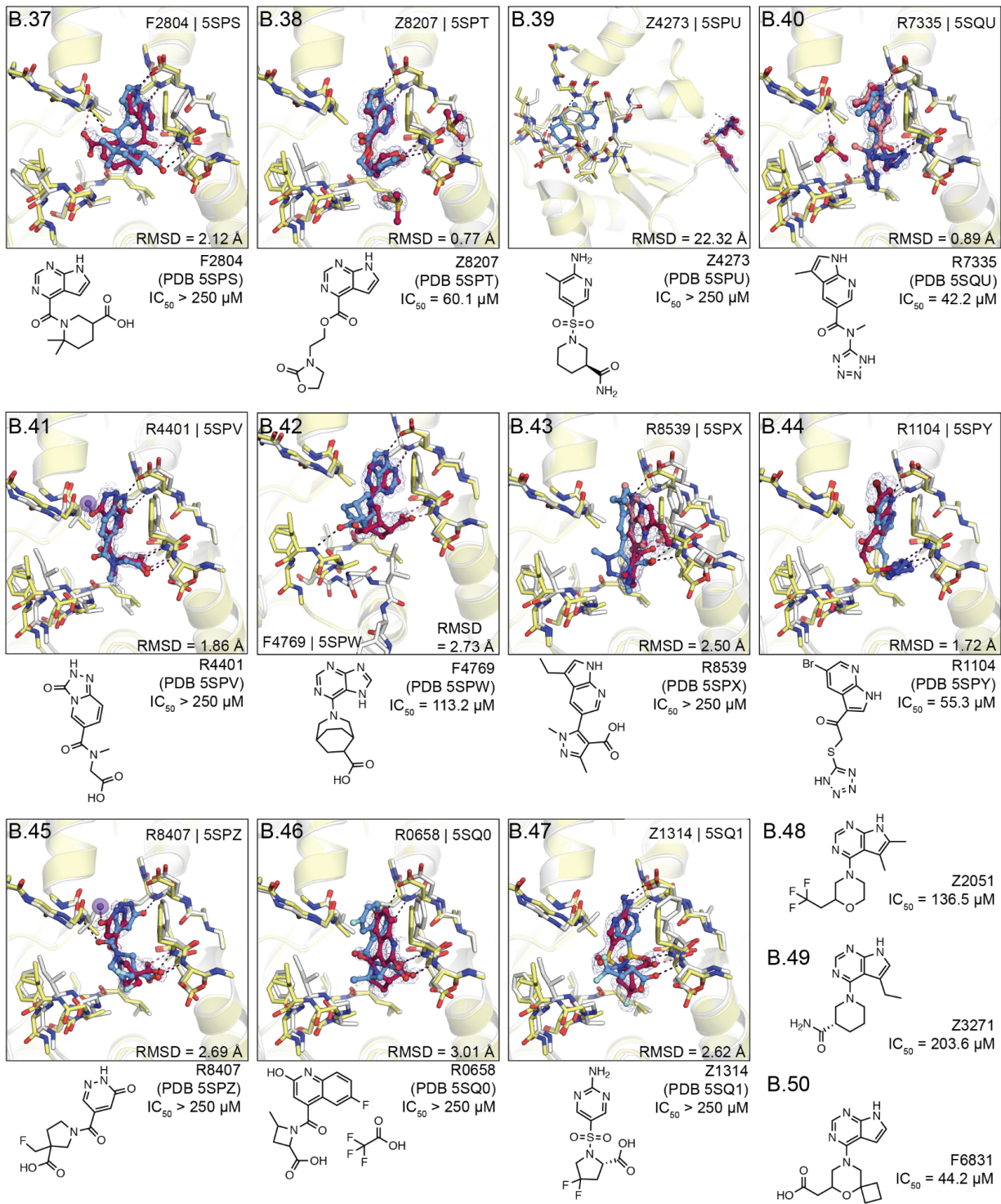


2<sup>nd</sup> Screen Docking Template

Docking Prediction

Crystal Structure

Solved Pose

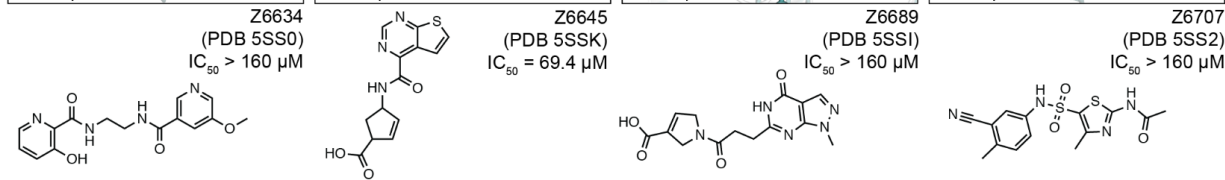
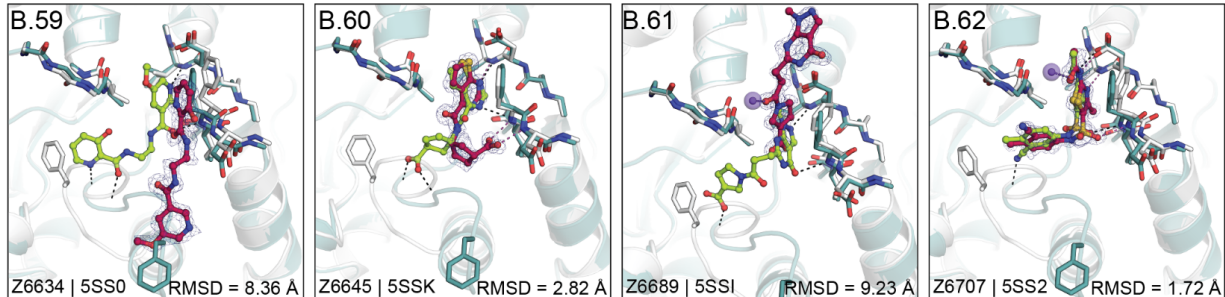
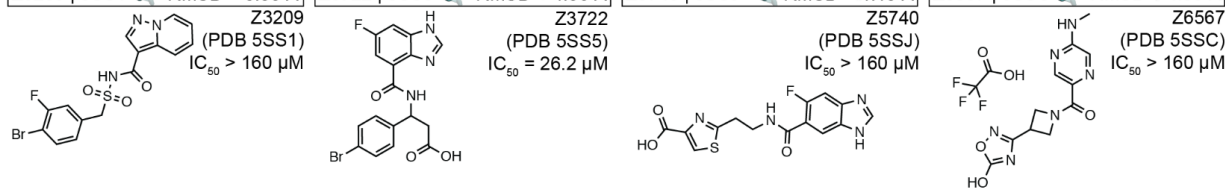
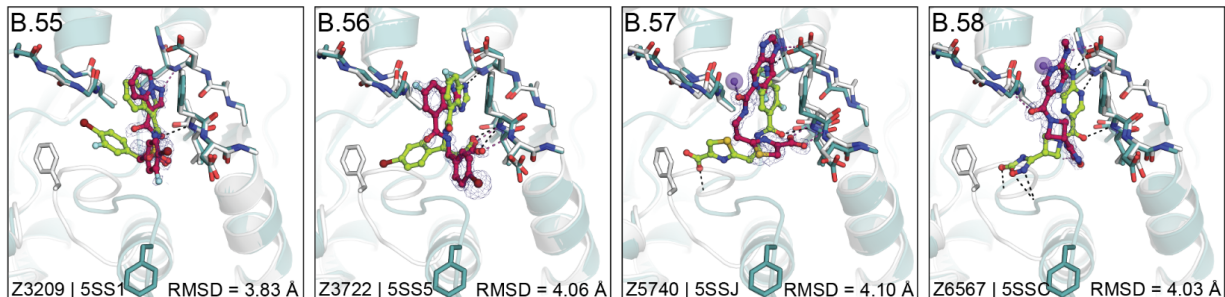
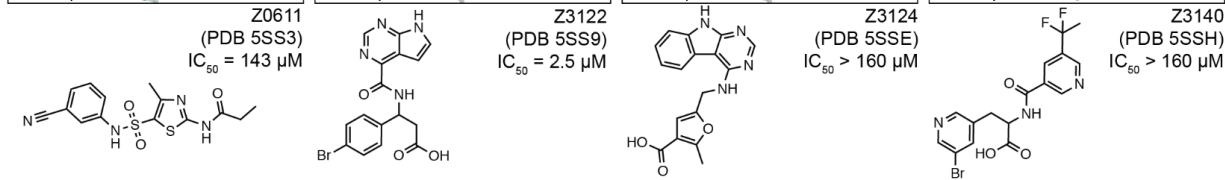
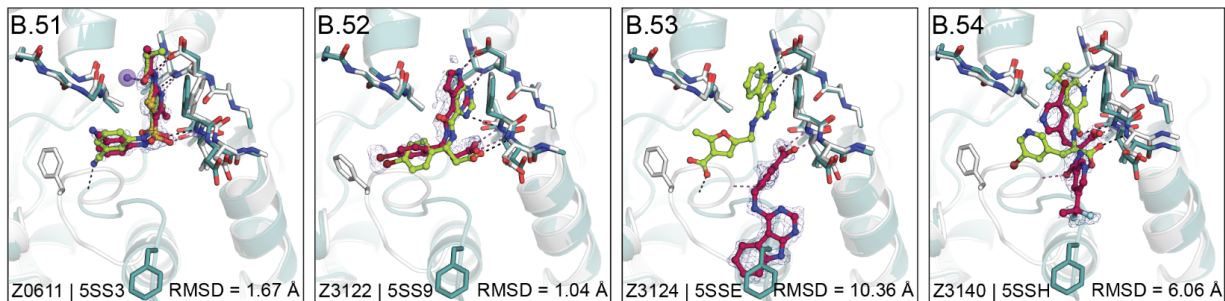


2<sup>nd</sup> Screen Docking Template

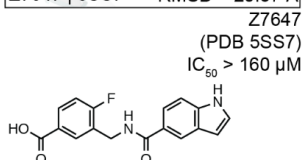
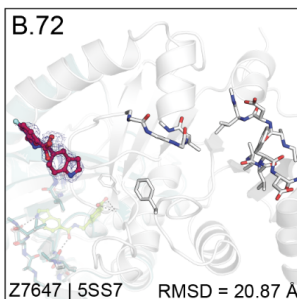
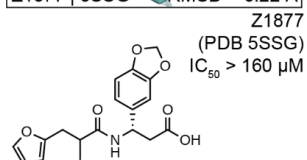
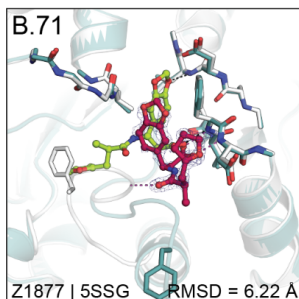
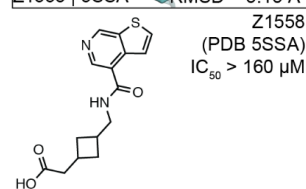
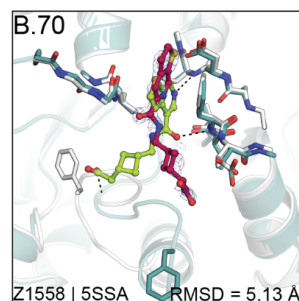
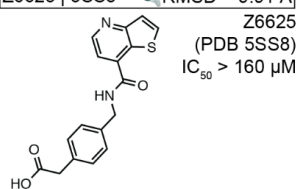
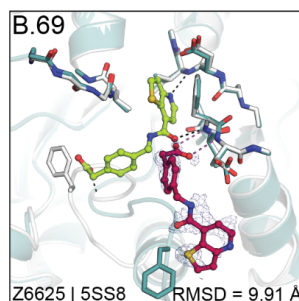
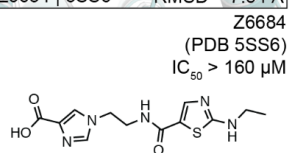
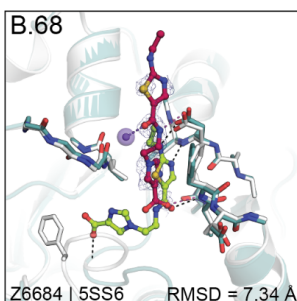
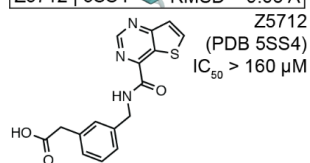
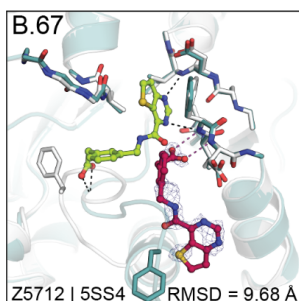
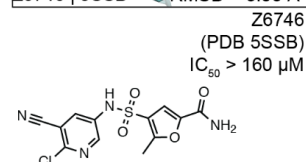
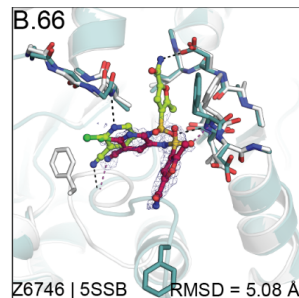
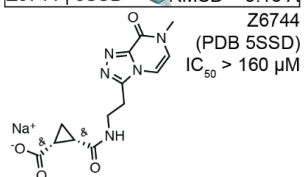
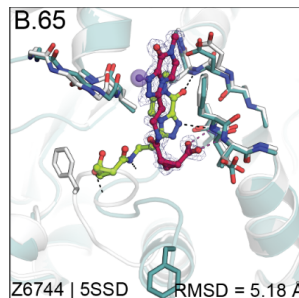
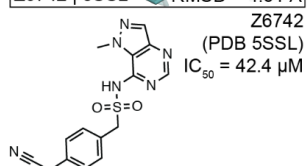
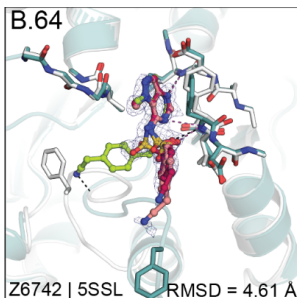
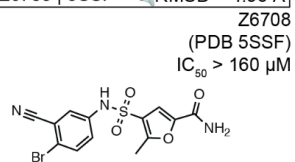
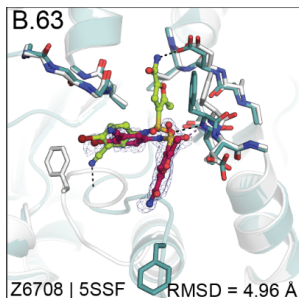
Docking Prediction

Crystal Structure

Solved Pose



Docking Template (open state)
Docking Prediction
Crystal Structure
Solved Pose



Docking Template (open state)

Docking Prediction

Crystal Structure

Solved Pose